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This work has given rise to significant advances in areas of mathematics and scientific computing closely related to some of the most important scientific and technology areas of our day. The time-domain solvers resulting from this effort hold a promise to raise the bar in time-domain solution of PDEs. The resulting Green function methods have provided a solution to the century-old Wood anomaly problem for the periodic Green function. Work on integral equations and solvers, in turn, has given rise to highly accurate solutions for some of the most challenging scattering problems in science and engineering.

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"High-Performance Computational Electromagnetics in Frequency-Domain and Time-Domain"

Final Report

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1 Introduction

This effort concerns development of *Highly accurate non-dispersive time-domain solvers for general domains* (Section 2); *Fast approaches for computation of periodic Green's functions* (Section 3); and *Integral equations and algorithms with high-quality spectral properties for problems involving combinations of perfect conductors and (lossy and loseless) penetrable scatterers* (Section 4). In the following sections we report on progress that has resulted from this effort in each one of these areas.

2 Time-domain Fourier-Continuation solvers

Significant progress occurred over the life of this contract in the area of FC (Fourier Continuation) methods for Partial Differential Equations in the time-domain [1–7]. Our efforts in these areas have resulted in explicit and implicit solvers for high- and low-frequency problems, for linear and nonlinear equations, and including media such as fluids, solids and vacuum—and combinations thereof. In each of the aforementioned publications a significant milestone was achieved. For example, the contributions [1, 7] provide methods that can be used to enable FC solution of nonlinear equations (such as the Burgers and Navier-Stokes equations) while maintaining high-order accuracy and dispersionlessness with *quasi-unconditional stability*: arbitrarily small values of Δx can be used for a fixed Δt, provided the Δt value adequately samples the problem. In the contribution [2], in turn, methods for FC solution of problems containing variable coefficients were introduced; in particular it was found that certain numerical boundary layers need to be adequately represented in order to ensure accurate solution. Reference [3] introduced an approach that allows for treatment of traction boundary conditions in wave propagation problems in solids [3, 4] (Navier's elastic wave equation) [1]. The thesis [5] uses the Fourier Continuation method in multiple ways: to solve equations, to propagate to distant regions without meshing, etc. The thesis additionally presented an implementation of a three-dimensional FC solver, hybridized with Discontinuous Galerkin, and fully implemented in a GPU computational infrastructure.

In all of these cases the FC method continued to display the excellent qualities observed previously in simpler contexts: high accuracy, exceptionally small dispersion and applicability to completely general configurations. As discussed in the aforementioned contributions, for a given

[1] In view of its applications to seismic wave propagation Dr. Amlani's PhD thesis received two awards at Caltech, one in our department and another one for which there is institute-wide competition. The second one is the Demetriades-Tsafka-Kokalis Prize in Engineering & Applied Science for best thesis, publication or discovery in seismo-engineering.

accuracy the FC method can be anywhere between hundreds and up to millions of times faster, for a given accuracy, than previous alternative solvers.[2] The new methods thus enable solution of previously intractable problems.

3 Periodic Green function

A number of contributions in the area of rough surfaces and periodic Green functions [8–11] over the span of this contract include use of a new "windowing" approach to greatly accelerate Green-function calculations [8], extension to periodic arrays of cylinders [9], introduction of acceleration in the periodic solver [10] and extension to three-dimensional periodic problems [11] as well as the novel construction, produced under sponsorship of this contract, of rapidly convergent periodic Green functions at Wood anomaly frequencies [8]. The latter problem is very well known and had defied solution since the early twentieth century. The new approach (which is based on use of finite-differences of shifted Green functions for acceleration of convergence even at Wood anomalies) greatly extends the applicability of the Green function methods for periodic scattering problems. The new method has maximum impact in three dimensional problems—for which Green function convergence can be extremely poor, as a result of the existence of large numbers of Wood frequencies. In all, progress in the area of rough surface scattering has been very significant, with applicability to problems in the general areas of metamaterials, oceanic scattering, light-coupling, etc.

4 Well-conditioned integral formulations and algorithms

Meaningful progress concerning well conditioned integral algorithms took place as a result of work sponsored by this contract, including rigorous mathematical theory and powerful numerical algorithms with applicability in a number of fields of science and engineering [12–21]. A variety of problems and configurations were thus considered, including problems of scattering by open surfaces [12–14]; improved integral methods for closed surfaces [15]; problems concerning propagation and scattering by penetrable scatterers [16]; studies of absorption properties of conducting materials containing asperities [17, 18]; as well as new methods for evaluation of Laplace eigenfunctions on general domains and under challenging boundary conditions [19, 20]. A rigorous convergence proof for the original methods [22] was provided in [21]. These contributions are discussed briefly in what follows.

An important project we considered during the span of this effort concerns the problem of scattering by open surfaces—the prototypical and simplest example of which is the infinitely thin perfectly-conducting disc. This problem has many applications in optics, from the very small to the very large (from nano-scale optical devices up and including the discovery of planets) as well as applications in stealth, antenna design, electronic and photonic devices, etc. For the first time a regularized integral equation yielding a Fredholm equation of the second kind for open-surface problems was put forth in the contributions [12–14], including rigorous analysis of the equations and efficient implementations in two- and three-dimensional space. In practice, the second-kind character of the equation enables solution by iterative solvers in very small numbers of iterations and it thus enables effective solution of the problem. The three-dimensional open-surface implementation provided in [12] is highly effective and sophisticated; using minimal iteration

[2] Examples which demonstrate such improvements in computing times in simple contexts are presented in [6]; comparative studies concerning the performance of the FC and other solvers in distributed-memory parallel infrastructures, on the other hand, can be found in [3, 5].

numbers[3] it can produce solution of scattering problems of very high accuracy. In a related effort, regularized integral equations and high-order solvers for sound-hard acoustic scattering problems were put forth in [15]; use of these equations gives rise to very significant improvements in iterations numbers over those required by the well known Burton-Miller formulation. The contribution [16], in turn, shows that these ideas can be ported successfully to the problem of penetrable scattering as well.

The contributions [17, 18] concern electromagnetic scattering by asperities (bumps or cavities) on otherwise undisturbed planar regions. Relying on use of Sommerfeld integrals we thus developed integral solvers which enable accurate evaluation of energy absorption for asperities of arbitrary shape. The contribution [17] is in fact much more general: in our method configurations are characterized by means of adequately selected structural elements so that physically diverse systems can be treated with minimal variations of a basic mathematical structure. Our studies of a variety of configurations [18] gave rise to interesting conclusions concerning the character of asperity-enhanced absorption. We found that typically absorption is enhanced by the presence of asperities, although, interestingly, absorption can also be significantly reduced in some cases—such as, e.g., in the case of a trench on a conducting plane where the incident electric field is perpendicular to the plane.

Consideration of various engineering and scientific configurations lead us to our recent development work concerning accurate numerical integral-equation methods for Laplace eigenvalue problems in general domains and under given boundary conditions [20]—with wide ranging applications in the fields of optics, photonics and antenna design, amongst many others, including analysis of waveguide and antenna problems. In particular this work provides a highly accurate eigensolver under the challenging *Zaremba* boundary conditions (for which no robust solvers existed before this work), and related Zaremba integral equation solvers [19] for the Helmholtz equation.

Rigorous proofs of existence, uniqueness and numerical stability are particularly useful in the context of integral equation methods, as they determine the conditions under which numerical solvers can be highly effective. Complete proofs of the well conditioned character of the aforementioned integral equation formulation for open surfaces was provided in [13, 14]. A numerical analysis of the related closed surface solvers [22], in turn, was for the first time put forth in [21]. We believe these two contributions contain a number of innovative theoretical elements which may prove valuable in the general theory of integral equations.

5 Conclusions

We believe this work has given rise to significant advances in areas of mathematics and scientific computing closely related to some of the most important scientific and technology areas of our day. The time-domain solvers mentioned in Section 2 hold a promise to raise the bar in time-domain solution of PDEs. The Green function methods mentioned in Section 3 have provided a solution to the century-old Wood anomaly problem for the periodic Green function. The work on integral equations and solver described in Section 4 has given rise to highly accurate solutions for some of the most challenging scattering problems in science and engineering. We look forward to future work that is at least as rewarding as the one described in this report.

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